# Macintosh HD:Users:simonem:MyResearch:DEPRO:HF(H2O)7:Fig-XH-Theta-hBondCompression.pdf

Figure 5: <i>z = <i, - i,>z is the conditional ensemble average at a given z value of the difference of the expectation value of the Kohn-Sham Hamiltonian computed over the two Maximally Localized Wannier Functions involved in each of the three hydrogen bonds forming the relevant H-bond chain (i,(r) = <i,(r) HKS(r)  i,(r)>, with  i,(x, r) denoting the -th Wannier function of the i-th H-bond). A negative (positive) value of <i>z means that the corresponding hydrogen is closer (more strongly bonded) to the heavy atom (F or O) it is bonded in the reactant (product) state. <i>z = 0 at the z-value at which the corresponding hydrogen is shared between the two heavy atoms. Arrows and lines are inserted to highlight the effect of the temperature on the z-value at which the various <i>z start to (significantly) change from their initial value (i.e. the corresponding hydrogen starts to migrate) or cross the zero.